



# A generic local thermal equilibrium model for porous reactive materials submitted to high temperatures



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## ARTICLE INFO

### Article history:

Received 8 May 2016

Received in revised form 13 October 2016

Accepted 21 November 2016

Available online 19 January 2017

### Keywords:

Porous media

High temperature

Chemistry

Pyrolysis

Transport

## ABSTRACT

Many engineering applications involve reacting porous materials submitted to high temperatures. This work presents a detailed but pragmatic heat and mass transfer model for porous materials containing several solid phases and a single gas phase. The detailed chemical interactions occurring between the solid phases and the gas phase are modeled at the pore scale assuming local thermal equilibrium. Homogenized models are obtained for solid pyrolysis, pyrolysis species injection in the gas phase, heterogeneous reactions between the solid phases and the gas phase, and homogeneous reactions in the gas phase. The chemistry models are integrated in a macroscopic model making use of volume-averaged governing equations for the conservation of solid mass, gas mass, species (finite-rate chemistry) or elements (equilibrium chemistry), momentum, and energy. The model has been implemented in the Porous Material Analysis Toolbox based on OpenFoam (PATO), distributed Open Source by NASA. Applications to two high-temperature engineering problems are presented. The first application concerns the design of heat-shields of space vehicles. The second one aims at improving the understanding of biomass pyrolysis for the production of biohydrocarbons.

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## 1. Introduction

Modeling of heat and mass transfer phenomena in porous materials is a complex and multifaceted topic. On the one hand, the scientific community has been able to experimentally infer and theoretically derive macroscopic models for simple situations. Darcy's law is a famous example. The direct proportionality between the mass flow rate and the pressure gradient of creeping flows in porous media was experimentally discovered by H. Darcy in the 19th century [1] and mathematically justified a couple of decades ago [2,3]. There is a rich literature of problems that have been understood, modeled using upscaling theories, and experimentally verified. They are now available in textbooks – for example, to cite a few of them: diffusion in porous media [4], convection in porous media [5], radiation in porous media [6]. Each particular field is the object of active research aiming at improving the theory for the derivation of macroscopic models and refining the experimental capabilities to measure parameters [7–10]. Computed

micro-tomography and direct numerical simulations (DNS) can, in some cases, usefully complement traditional upscaling and experimental analyses [8,11,12]. On the other hand, there is a large range of complex multi-physics problems for which detailed mathematical derivations lead to non-practical models and experimental or DNS analyses are difficult. Models are therefore either empirical, heuristic, or based on an upscaling theory with some assumptions, typically neglecting couplings between most phenomena for practical reasons. This is in particular the case for reactive porous materials submitted to high-temperatures. Typical high-temperature engineering applications involving chemical reactions are heat shields of space vehicles using ablative materials [13–15] or transpiration cooling [16], nozzle's walls of rockets [17–19], carbonization of pyrolyzing porous materials like biomass [20–23], cracking of hot gases passing through a porous material [24–26], chemical vapor infiltration and deposition [27,28], . . . , to simple burning of a match.

From a material point of view, there are more similarities than differences between the applications cited, even between the porous heat-shield of a space vehicle entering an atmosphere at hypersonic speed and a match burning (Fig. 1). In most cases,

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## Nomenclature

### Latin

$c_p$	specific heat, $J \cdot kg^{-1} \cdot K^{-1}$
$A_i$	species $i$
$A_{i,j}$	Arrhenius law pre-exponential factor, $SI$
$e$	specific energy, $J \cdot kg^{-1}$
$\mathcal{E}_{i,j}$	Arrhenius law activation energy, $J \cdot mol^{-1}$
$\mathcal{F}$	effective diffusion flux, $kg \cdot m^{-2} \cdot s^{-1}$
$F_{i,j}$	fraction of subphase $j$ in phase $i$
$h$	specific absolute enthalpy, $J \cdot kg^{-1}$
$\underline{\mathbf{K}}$	permeability tensor, $m^2$
$\underline{\underline{\mathbf{k}}}$	conductivity tensor, $J \cdot m^{-2} \cdot s^{-1} \cdot K^{-1}$
$\underline{\underline{k}}_r$	reaction rates, $SI$
$\mathcal{M}$	molar mass, $kg \cdot mol^{-1}$
$m_{i,j}$	Arrhenius law parameter
$n_{i,j}$	Arrhenius law parameter
$N_g$	number of gaseous species
$N_p$	number of solid phases
$p$	pressure, Pa
$P_i$	number of subphases in solid phase $i$
$Q$	effective diffusion heat flux, $J \cdot m^{-2} \cdot s^{-1}$
$\mathcal{R}$	perfect gas constant, $J \cdot mol^{-1} \cdot K^{-1}$
$s$	specific surface, $m^2 \cdot m^{-3}$
$\mathbf{v}$	convection velocity, $m \cdot s^{-1}$
$\mathbf{x}, \mathbf{y}$	space variables, respectively macroscopic and local.
$X$	molar density, $mol \cdot m^{-3}$
$y$	species mass fractions
$z$	element mass fractions

### Greek

$\beta$	Klinkenberg tensor, Pa
$\bar{\epsilon}$	volume fraction
$\eta$	tortuosity
$\zeta$	mass stoichiometric coefficient
$\theta$	active site density, $mol \cdot m^{-3}$
$\mu$	viscosity, $Pa \cdot s$
$\nu$	stoichiometric coefficients
$\Pi$	pyrolysis gas production rate, $kg \cdot m^{-3} \cdot s^{-1}$
$\pi_k$	pyrolysis production rate of species/element $k$ , $kg \cdot m^{-3} \cdot s^{-1}$
$\rho$	density, $kg \cdot m^{-3}$
$\chi_{i,j}$	advancement of pyrolysis reaction $j$ within phase $i$
$\psi$	generic variable
$\omega$	production rate, $mol \cdot m^{-3} \cdot s^{-1}$
$\Omega_h$	overall heterogeneous mass reaction rate, $kg \cdot m^{-3} \cdot s^{-1}$
$\omega_i^h$	effective heterogeneous mass reaction rate of phase $i$ , $kg \cdot m^{-3} \cdot s^{-1}$

### Subscripts

$g$	Gas phase
$p$	Solid phase
$t$	Solid and gas phases

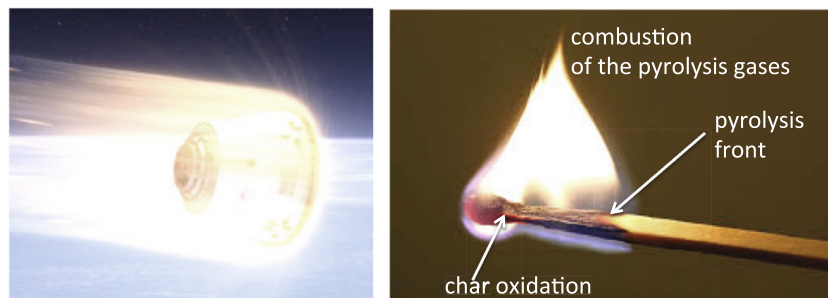
external flow conditions only affect the internal behavior of a porous material through boundary conditions at the material/environment interface. The conservation laws within the materials are essentially the same and the same mathematical model may be used to analyze their behaviors. In the literature, we find different types of notations and simplifying hypotheses for the different applications but they rely on the same physics and base model, with of course sometimes additional features required for some applications. The motivation of this article is to provide a detailed physics-based framework for engineering analyses and simulations. It contains all the base features needed to model the high-temperature applications mentioned, with a special effort to detail the chemistry. The following heat and mass transport phenomena are modeled: pyrolysis, pyrolysis species production, homogeneous and heterogeneous reactions (equilibrium or finite-rate), species transport by convection and diffusion, momentum conservation in porous media, and energy conservation. To keep the model generic and pragmatic, we assume local thermal equilibrium and local chemical homogeneity in the gas phase. A

numerical simulation tool implementing this model is released open source.

The article is organized as follows. In section two, we present a generic local thermal equilibrium model for decomposing and reacting porous materials, containing several solid phases and a single gas phase in the continuum regime (small Knudsen number). In section three, the model capabilities are illustrated with the analysis of two diverse applications. The first one concerns the analysis of the thermal response of the ablative heat-shield of a space vehicle. The second one aims at improving the understanding of biomass pyrolysis for the production of green energy. Section four provides a summary and points the reader to an implementation of the formulation available open source.

## 2. Model

In this section, we present a generic local thermal equilibrium model for decomposing and reacting porous materials, containing several solid phases and a single gas phase. The governing



a) atmospheric entry of a space vehicle (high-temperature, high-speed flow) b) match burning

Fig. 1. Two high-temperature reactive porous medium applications.

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